



## Thermophoresis of water droplets inside carbon nanotubes

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*Published in:*  
Bulletin of the American Physical Society

*Publication date:*  
2016

*Document Version*  
Peer reviewed version

[Link back to DTU Orbit](#)

*Citation (APA):*  
Zambrano, H., Walther, J. H., Oyarzua, E., & Rojano, A. (2016). Thermophoresis of water droplets inside carbon nanotubes. In *Bulletin of the American Physical Society* (Vol. 61). [E22.00006 ] American Physical Society.

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Abstract Submitted  
for the DFD16 Meeting of  
The American Physical Society

Sorting Category: 25.1 (C)

**Thermophoresis of water droplets inside carbon nanotubes**<sup>1</sup> HARVEY ZAMBRANO, University of Concepcion, JH WALTHER<sup>2</sup>, Technical University of Denmark, ELTON OYARZUA, ANDRES ROJANO, University of Concepcion — Carbon Nanotubes (CNTs) offer unique possibilities as fluid conduits with applications ranging from lab on a chip devices to encapsulation media for drug delivery. CNTs feature high mechanical strength, chemical and thermal stability and biocompatibility therefore they are promising candidates for nanodevice fabrication. Thermal gradients have been proposed as mechanism to drive particles, fullerenes and droplets inside CNTs. Here, by conducting Molecular Dynamics (MD) simulations, we study thermophoresis of water droplets inside CNTs. We systematically change the size of the droplets, the axial thermal gradient and CNT chirality. We find that the droplet motion in the armchair CNTs exhibits two clearly delimited stages, a regime wherein the droplet is accelerated and subsequently, a regime wherein the droplet moves with constant velocity. Inside the zig zag CNTs, the droplet accelerates during a very short time and then it moves with constant velocity. We compute the net force during the droplet acceleration and find a correlation between the droplet acceleration and the magnitude of the thermal gradient without any dependence on the droplet size. Moreover, we conduct velocity constrained MD simulations to determine the friction and thermophoretic forces acting on the droplet.

<sup>1</sup>We acknowledge partial funding from FONDECYT through the project No. 11130559 and from VRID Universidad de Concepcion.

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☒ Prefer Oral Session  
☐ Prefer Poster Session

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Date submitted: 01 Aug 2016

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